Supplemental material

Carbon Cluster Formation during Thermal Decomposition of HMX and TATB High Explosives from ReaxFF Reactive Molecular Dynamics Simulations

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The complete set of ReaxFF reactive force field parameters used in this paper organized in a form appropriate for input to the ReaxFF reactive dynamics program [Ref. 1].

```
Reactive MD-force field: nitramines (RDX/HMX/TATB/PETN)
 39       ! Number of general parameters
   50.0000 !Overcoordination parameter
    9.4514 !Overcoordination parameter
   30.0000 !Valency angle conjugation parameter
  216.4305 !Triple bond stabilisation parameter
   12.4838 !Triple bond stabilisation parameter
    0.0000 !C2-correction
    1.0701 !Undercoordination parameter
    7.5000 !Triple bond stabilisation parameter
   11.9083 !Undercoordination parameter
   13.3822 !Undercoordination parameter
  -10.4637 !Triple bond stabilization energy
    0.0000 !Lower Taper-radius
   10.0000 !Upper Taper-radius
    2.8793 !Not used
   33.8667 !Valency undercoordination
    3.5895 !Valency angle/lone pair parameter
    1.0563 !Valency angle
    2.0384 !Valency angle parameter
    6.1431 !Not used
    6.9290 !Double bond/angle parameter
    0.0283 !Double bond/angle parameter: overcoord
    0.0570 !Double bond/angle parameter: overcoord
   -2.4837 !Not used
    5.8374 !Torsion/BO parameter
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```
   10.0000 !Torsion overcoordination
    1.8820 !Torsion overcoordination
   -1.2327 !Conjugation 0 (not used)
    2.1861 !Conjugation
    1.5591 !vdWaals shielding
    0.0100 !Cutoff for bond order (*100)
    5.2216 !Valency angle conjugation parameter
    3.4021 !Overcoordination parameter
   38.5241 !Overcoordination parameter
    2.1533 !Valency/lone pair parameter
    0.5000 !Not used
   20.0000 !Not used
    5.0000 !Molecular energy (not used)
    0.0000 !Molecular energy (not used)
    6.5560 !Valency angle conjugation parameter
  7    ! Nr of atoms; cov.r;
valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
            alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.
            cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.
            ov/un;val1;n.u.;val3,vval4
 C    1.3742   4.0000  12.0000   1.9684   0.1723   0.8712
1.2385   4.0000
      9.4606   2.1346   4.0000  31.0823  79.5548   5.7254
6.9235   0.0000
      1.2104   0.0000 183.7012   5.7419  33.3951  11.9957
0.8563   0.0000
     -2.8983   2.5000   1.0564   4.0000   2.9663   0.0000
0.0000   0.0000
 H    0.6867   1.0000   1.0080   1.3525   0.0616   0.8910  -
0.1000   1.0000
      9.3858   5.0013   1.0000   0.0000 121.1250   3.8446
10.0839   1.0000
     -0.1000   0.0000  58.4228   3.8461   3.2540   1.0000
1.0698   0.0000
    -15.7683   2.1504   1.0338   1.0000   2.8793   0.0000
0.0000   0.0000
 O    1.3142   2.0000  15.9990   1.9741   0.0880   0.8712
1.1139   6.0000
     10.2186   7.7719   4.0000  29.5271 116.0768   8.5000
7.1412   2.0000
      0.9909  14.9473  69.2812   9.1371   1.6258   0.1863
0.9745   0.0000
     -3.5965   2.5000   1.0493   4.0000   2.9225   0.0000
0.0000   0.0000
 N    1.2450   3.0000  14.0000   1.9951   0.1088   1.0512
1.1911   5.0000
```

```
      9.9303   7.8431   4.0000  32.4758 100.0000   6.7768
6.8035   2.0000
      1.0636   0.1045 128.0119   2.1604   2.9464   2.5181
0.9745   0.0000
     -4.0959   2.0047   1.0183   4.0000   2.8793   0.0000
0.0000   0.0000
 S    1.9647   2.0000  32.0600   2.0783   0.2176   1.0336
1.5386   6.0000
      9.9676   5.0812   4.0000  35.1648 112.1416   6.5000
8.2545   2.0000
      1.4703   9.4922  70.0338   8.5146  28.0801   8.5010
0.9745   0.0000
    -10.0773   2.7466   1.0338   6.2998   2.8793   0.0000
0.0000   0.0000
 Si   2.0276   4.0000  28.0600   2.2042   0.1322   0.8218
1.5758   4.0000
     11.9413   2.0618   4.0000  11.8211 136.4845   1.8038
7.3852   0.0000
     -1.0000   0.0000 126.5331   6.4918   8.5961   0.2368
0.8563   0.0000
     -3.8112   3.1873   1.0338   4.0000   2.5791   0.0000
0.0000   0.0000
 X   -0.1000   2.0000   1.0080   2.0000   0.0000   1.0000  -
0.1000   6.0000
     10.0000   2.5000   4.0000   0.0000   0.0000   8.5000
1.5000   0.0000
     -0.1000   0.0000  -2.3700   8.7410  13.3640   0.6690
0.9745   0.0000
    -11.0000   2.7466   1.0338   4.0000   2.8793   0.0000
0.0000   0.0000
 18      ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                         pbe2;pbo3;pbo4;Etrip;pbo1;pbo2;ovcorr
  1  1 141.9346 113.4487  67.6027   0.1554  -0.3045   1.0000
30.4515   0.4283
         0.0801  -0.2113   8.5395   1.0000  -0.0933   6.6967
1.0000   0.0000
  1  2 163.6889   0.0000   0.0000  -0.4525   0.0000   1.0000
6.0000   0.5921
        12.1053   1.0000   0.0000   1.0000  -0.0097   8.6351
0.0000   0.0000
  2  2 169.8421   0.0000   0.0000  -0.3591   0.0000   1.0000
6.0000   0.7503
         9.3119   1.0000   0.0000   1.0000  -0.0169   5.9406
0.0000   0.0000
  1  3 164.0476 117.4881  72.1261  -0.6031  -0.1795   1.0000
14.9755   0.5413
```

```
         1.2626  -0.3063   7.0000   1.0000  -0.1588   4.5000
0.0000   0.0000
  3  3 110.4748 155.6441  40.0000   0.1150  -0.1054   1.0000
28.5221   0.2000
         0.9590  -0.2635   8.5715   1.0000  -0.1007   6.8548
1.0000   0.0000
  1  4 130.7147 175.2276  97.2523  -0.0368  -0.4942   1.0000
26.7545   0.5133
         0.3296  -0.3653   7.0000   1.0000  -0.1171   5.1025
1.0000   0.0000
  3  4  85.4950 114.0081  70.1453   0.5778  -0.1070   1.0000
16.6611   0.2339
         0.3474  -0.1948   8.3762   1.0000  -0.1089   5.8148
1.0000   0.0000
  4  4 157.7518  67.1322 160.9732  -0.5869  -0.1824   1.0000
12.0000   0.7136
         0.8204  -0.1657  10.6490   1.0000  -0.0967   4.5976
1.0000   0.0000
  2  3 224.3076   0.0000   0.0000  -0.6280   0.0000   1.0000
6.0000   1.0000
         5.0050   1.0000   0.0000   1.0000  -0.0512   5.1982
0.0000   0.0000
  2  4 212.1772   0.0000   0.0000  -0.3585   0.0000   1.0000
6.0000   0.3316
        10.4316   1.0000   0.0000   1.0000  -0.0658   6.4545
0.0000   0.0000
  1  5 128.7959  56.4134  39.0716   0.0688  -0.4463   1.0000
31.1766   0.4530
         0.1955  -0.3587   6.2148   1.0000  -0.0770   6.6386
1.0000   0.0000
  2  5 128.6090   0.0000   0.0000  -0.5555   0.0000   1.0000
6.0000   0.4721
        10.8735   1.0000   0.0000   1.0000  -0.0242   9.1937
1.0000   0.0000
  3  5   0.0000   0.0000   0.0000   0.5563  -0.4038   1.0000
49.5611   0.6000
         0.4259  -0.4577  12.7569   1.0000  -0.1100   7.1145
1.0000   0.0000
  4  5   0.0000   0.0000   0.0000   0.4438  -0.2034   1.0000
40.3399   0.6000
         0.3296  -0.3153   9.1227   1.0000  -0.1805   5.6864
1.0000   0.0000
  5  5  96.1871  93.7006  68.6860   0.0955  -0.4781   1.0000
17.8574   0.6000
         0.2723  -0.2373   9.7875   1.0000  -0.0950   6.4757
1.0000   0.0000
```

```
  6  6 109.1904  70.8314  30.0000   0.2765  -0.3000   1.0000
16.0000   0.1583
         0.2804  -0.1994   8.1117   1.0000  -0.0675   8.2993
0.0000   0.0000
  2  6 137.1002   0.0000   0.0000  -0.1902   0.0000   1.0000
6.0000   0.4256
        17.7186   1.0000   0.0000   1.0000  -0.0377   6.4281
0.0000   0.0000
  3  6 191.1743  52.0733  43.3991  -0.2584  -0.3000   1.0000
36.0000   0.8764
         1.0248  -0.3658   4.2151   1.0000  -0.5004   4.2605
1.0000   0.0000
 10    ! Nr of off-diagonal terms;
Ediss;Ro;gamma;rsigma;rpi;rpi2
  1  2   0.0464   1.8296  10.1311   1.0029  -1.0000  -1.0000
  2  3   0.0375   1.7275  10.8037   0.8813  -1.0000  -1.0000
  2  4   0.0509   1.7672  10.4261   0.9990  -1.0000  -1.0000
  1  3   0.1036   1.8869   9.5668   1.3590   1.1099   1.1534
  1  4   0.1971   1.7356  10.0734   1.2754   1.2113   1.1172
  3  4   0.0535   1.6709  10.8180   1.2968   1.1416   1.0167
  2  6   0.0470   1.6738  11.6877   1.1931  -1.0000  -1.0000
  3  6   0.1263   1.8163  10.6833   1.6266   1.2052  -1.0000
  1  5   0.1408   1.8161   9.9393   1.7986   1.3021   1.4031
  2  5   0.0895   1.6239  10.0104   1.4640  -1.0000  -1.0000
 62    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
  1  1  1  74.0317  32.2712   0.9501   0.0000   0.1780  10.5736
1.0400
  1  1  2  70.6558  14.3658   5.3224   0.0000   0.0058   0.0000
1.0400
  2  1  2  76.7339  14.4217   3.3631   0.0000   0.0127   0.0000
1.0400
  1  2  2   0.0000   0.0000   6.0000   0.0000   0.0000   0.0000
1.0400
  1  2  1   0.0000   3.4110   7.7350   0.0000   0.0000   0.0000
1.0400
  2  2  2   0.0000  27.9213   5.8635   0.0000   0.0000   0.0000
1.0400
  1  1  3  65.3104   6.3897   7.5000   0.0000   0.2000  10.0000
1.8525
  3  1  3  71.9855  28.5708   6.4252   0.0000   0.2000   0.0000
1.8525
  1  1  4  65.8892  45.0000   1.6598   0.0000   0.2000  10.0000
1.8525
  3  1  4  73.1057  25.8227   4.2145   0.0000   0.2000   0.0000
1.8525
  4  1  4  65.8759  40.9838   2.4369   0.0000   0.2000   0.0000
1.8525
```

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  2  1  3  56.3039  17.3681   5.3095   0.0000   0.9110   0.0000
1.0400
  2  1  4  71.5505  11.1820   3.7129   0.0000   0.9110   0.0000
1.0400
  1  2  4   0.0000   0.0019   6.3000   0.0000   0.0000   0.0000
1.0400
  1  3  1  72.3642  37.8942   1.1566   0.0000   0.7472   0.0000
1.2639
  1  3  3  90.0000  45.0000   0.5719   0.0000   0.7472   0.0000
1.2639
  1  3  4  70.4313  14.4055   7.1593   0.0000   0.7472   0.0000
1.2639
  3  3  3  83.8833  23.3345   2.3433 -10.0000   0.7472   0.0000
1.2639
  3  3  4  84.0407  45.0000   1.0695   0.0000   0.7472   0.0000
1.2639
  4  3  4  73.9966  24.4410   5.2760   0.0000   0.7472   0.0000
1.2639
  1  3  2  89.1394  37.0874   0.3849   0.0000   3.0000   0.0000
1.2618
  2  3  3  80.7068   5.0854   5.7151   0.0000   3.0000   0.0000
1.2618
  2  3  4  76.0238  45.0000   0.8637   0.0000   3.0000   0.0000
1.2618
  2  3  2  82.3474  13.5165   3.4896   0.0000   0.3596   0.0000
1.3307
  1  4  1  68.4330  19.3525   2.1625   0.0000   1.7325   0.0000
1.0440
  1  4  3  86.2893  37.5587   1.2660   0.0000   1.7325   0.0000
1.0440
  1  4  4  74.2404  12.0547   7.5000   0.0000   1.7325   0.0000
1.0440
  3  4  3  78.5566  43.8492   1.3351 -26.1471   1.7325  40.0000
1.0440
  3  4  4  77.4239  33.7297   1.7944  -0.9193   1.7325   0.0000
1.0440
  4  4  4  64.9107  17.5558   7.5000   0.0000   1.7325   0.0000
1.0440
  1  4  2  90.0000  32.0540   0.7195   0.0000   0.5355   0.0000
2.5279
  2  4  3  84.1185  45.0000   1.3826   0.0000   0.5355   0.0000
2.5279
  2  4  4  78.7133  24.6250   3.8202   0.0000   0.5355   0.0000
2.5279
  2  4  2  56.3036  14.1532   3.3914   0.0000   0.2000   0.0000
2.1689
```

```
  1  2  3   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000
1.0400
  1  2  4   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000
1.0400
  1  2  5   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000
1.0400
  3  2  3   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000
1.0400
  3  2  4   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000
1.0400
  4  2  4   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000
1.0400
  2  2  3   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000
1.0400
  2  2  4   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000
1.0400
  1  1  5  74.4180  33.4273   1.7018   0.1463   0.5000   0.0000
1.6178
  1  5  1  79.7037  28.2036   1.7073   0.1463   0.5000   0.0000
1.6453
  2  1  5  63.3289  29.4225   2.1326   0.0000   0.5000   0.0000
3.0000
  1  5  2  85.9449  38.3109   1.2492   0.0000   0.5000   0.0000
1.1000
  1  5  5  85.6645  40.0000   2.9274   0.1463   0.5000   0.0000
1.3830
  2  5  2  83.8555   5.1317   0.4377   0.0000   0.5000   0.0000
3.0000
  2  5  5  97.0064  32.1121   2.0242   0.0000   0.5000   0.0000
2.8568
  6  6  6  69.3456  21.7361   1.4283   0.0000  -0.2101   0.0000
1.3241
  2  6  6  75.6168  21.5317   1.0435   0.0000   2.5179   0.0000
1.0400
  2  6  2  78.3939  20.9772   0.8630   0.0000   2.8421   0.0000
1.0400
  3  6  6  70.3016  15.4081   1.3267   0.0000   2.1459   0.0000
1.0400
  2  6  3  73.8232  16.6592   3.7425   0.0000   0.8613   0.0000
1.0400
  3  6  3  90.0344   7.7656   1.7264   0.0000   0.7689   0.0000
1.0400
  6  3  6  22.1715   3.6615   0.3160   0.0000   4.1125   0.0000
1.0400
  2  3  6  83.7634   5.6693   2.7780   0.0000   1.6982   0.0000
1.0400
```

```
  3  3  6  73.4663  25.0761   0.9143   0.0000   2.2466   0.0000
1.0400
  2  2  6   0.0000  47.1300   6.0000   0.0000   1.6371   0.0000
1.0400
  6  2  6   0.0000  31.5209   6.0000   0.0000   1.6371   0.0000
1.0400
  3  2  6   0.0000  31.0427   4.5625   0.0000   1.6371   0.0000
1.0400
  2  2  5   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000
1.0400
 23    ! Nr of
torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
  1  1  1  1   0.0000  48.4194   0.3163  -8.6506  -1.7255
0.0000   0.0000
  1  1  1  2   0.0000  63.3484   0.2210  -8.8401  -1.8081
0.0000   0.0000
  2  1  1  2   0.0000  45.2741   0.4171  -6.9800  -1.2359
0.0000   0.0000
  0  1  2  0   0.0000   0.0000   0.0000   0.0000   0.0000
0.0000   0.0000
  0  2  2  0   0.0000   0.0000   0.0000   0.0000   0.0000
0.0000   0.0000
  0  1  3  0  -0.0002  85.8794   0.3236  -3.8134  -2.0000
0.0000   0.0000
  0  2  3  0   0.0000   0.1000   0.0200  -2.5415   0.0000
0.0000   0.0000
  0  3  3  0  -0.9667 116.4743   0.0002  -4.9422   0.0000
0.0000   0.0000
  0  1  4  0  -0.0069 150.0000   0.4891  -7.4921  -2.0000
0.0000   0.0000
  0  2  4  0   0.0000   0.1000   0.0200  -2.5415   0.0000
0.0000   0.0000
  0  3  4  0   1.6745  56.6301  -0.0008  -4.5064  -2.0000
0.0000   0.0000
  0  4  4  0   1.1253  75.3447   0.0080  -9.0000  -2.0000
0.0000   0.0000
  0  1  1  0   0.0930  18.5962   0.0002  -9.0000  -1.0000
0.0000   0.0000
  4  1  4  4  -2.0000  20.8732  -1.5000  -9.0000  -2.0000
0.0000   0.0000
  0  1  5  0   4.0885  78.7058   0.1174  -2.1639   0.0000
0.0000   0.0000
  0  5  5  0  -0.0170 -56.0786   0.6132  -2.2092   0.0000
0.0000   0.0000
  0  2  5  0   0.0000   0.0000   0.0000   0.0000   0.0000
0.0000   0.0000
```

```
  0  6  6  0   0.0000   0.0000   0.1200  -2.4426   0.0000
0.0000   0.0000
  0  2  6  0   0.0000   0.0000   0.1200  -2.4847   0.0000
0.0000   0.0000
  0  3  6  0   0.0000   0.0000   0.1200  -2.4703   0.0000
0.0000   0.0000
  1  1  3  3  -0.0002  21.5452   0.1727  -9.0000  -2.0000
0.0000   0.0000
  1  3  3  1   0.0002  79.3777  -1.5000  -5.2139  -2.0000
0.0000   0.0000
  3  1  3  3  -1.3476  22.4932   1.5000  -9.0000  -2.0000
0.0000   0.0000
  9    ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
  3  2  3   2.0000  -5.0000   3.0000   3.0000
  3  2  4   1.7753  -5.0000   3.0000   3.0000
  4  2  3   1.3884  -5.0000   3.0000   3.0000
  4  2  4   1.6953  -4.0695   3.0000   3.0000
  3  2  5   2.6644  -3.0000   3.0000   3.0000
  4  2  5   4.0476  -3.0000   3.0000   3.0000
  5  2  3   2.1126  -4.5790   3.0000   3.0000
  5  2  4   2.2066  -5.7038   3.0000   3.0000
  5  2  5   1.9461  -4.0000   3.0000   3.0000
```